



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:35 AM GMT

PDB ID : 2J9F
Title : HUMAN BRANCHED-CHAIN ALPHA-KETOACID DEHYDROGENASE-
DECARBOXYLASEE1B
Authors : Jun, L.; Machius, M.; Chuang, J.L.; Wynn, R.M.; Chuang, D.T.
Deposited on : 2006-11-07
Resolution : 1.88 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

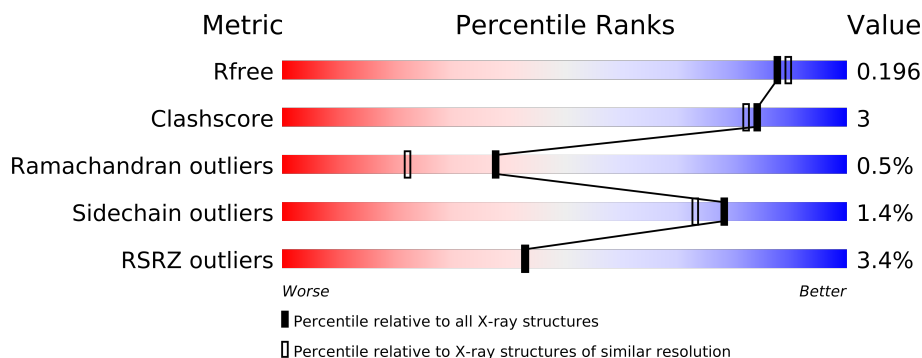
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	5260 (1.90-1.86)
Clashscore	79885	6268 (1.90-1.86)
Ramachandran outliers	78287	6195 (1.90-1.86)
Sidechain outliers	78261	6196 (1.90-1.86)
RSRZ outliers	66119	5262 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	400	
1	C	400	
2	B	350	
2	D	350	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	D	1345	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12596 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	9	0
			3135	1972	559	585	19			
1	C	383	Total	C	N	O	S	0	9	0
			3143	1977	565	584	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	PRO	SER	ENGINEERED MUTATION	UNP P12694
C	302	PRO	SER	ENGINEERED MUTATION	UNP P12694

- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	5	1
			2597	1672	428	482	15			
2	D	330	Total	C	N	O	S	0	1	1
			2566	1652	423	476	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	343	GLY	-	EXPRESSION TAG	UNP P21953
B	344	GLY	-	EXPRESSION TAG	UNP P21953
B	345	HIS	-	EXPRESSION TAG	UNP P21953
B	346	HIS	-	EXPRESSION TAG	UNP P21953
B	347	HIS	-	EXPRESSION TAG	UNP P21953
B	348	HIS	-	EXPRESSION TAG	UNP P21953
B	349	HIS	-	EXPRESSION TAG	UNP P21953
B	350	HIS	-	EXPRESSION TAG	UNP P21953

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	343	GLY	-	EXPRESSION TAG	UNP P21953
D	344	GLY	-	EXPRESSION TAG	UNP P21953
D	345	HIS	-	EXPRESSION TAG	UNP P21953
D	346	HIS	-	EXPRESSION TAG	UNP P21953
D	347	HIS	-	EXPRESSION TAG	UNP P21953
D	348	HIS	-	EXPRESSION TAG	UNP P21953
D	349	HIS	-	EXPRESSION TAG	UNP P21953
D	350	HIS	-	EXPRESSION TAG	UNP P21953

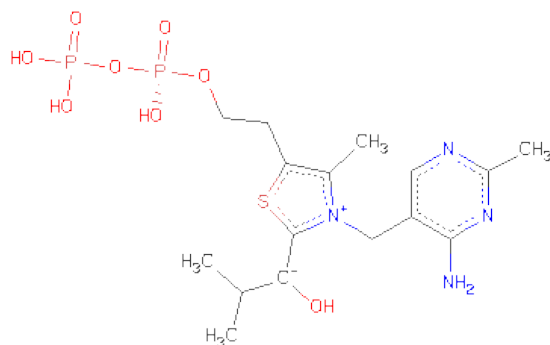
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total K 1 1	0	0
4	A	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is C2-1-HYDROXY-3-METHYL-PROPYL-THIAMINDIPHOSPHATE (three-letter code: THV) (formula: C₁₆H₂₆N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	16	4	8	2	1		
5	C	1	Total	C	N	O	P	S	0	0
			31	16	4	8	2	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

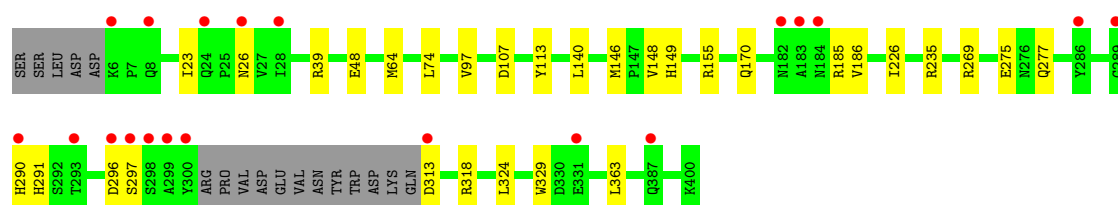
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	291	Total	O	0	0
			291	291		
7	B	243	Total	O	0	0
			243	243		
7	C	297	Total	O	0	0
			297	297		
7	D	238	Total	O	0	0
			238	238		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

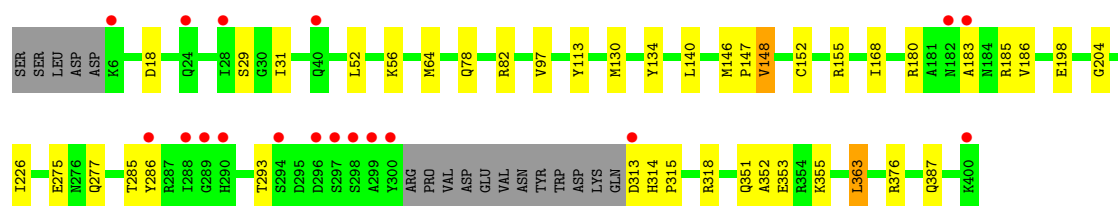
• Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT

Chain A: 



• Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT

Chain C: 



• Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT

Chain B: 



• Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.34Å 145.34Å 138.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.64 – 1.88 26.64 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.64-1.88) 99.2 (26.64-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.200 0.171 , 0.196	Depositor DCC
R_{free} test set	1491 reflections (1.12%)	DCC
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.0	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 135010 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.53 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6991e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, MN, THV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.66	0/3211	0.76	1/4336 (0.0%)
1	C	0.66	0/3219	0.77	2/4345 (0.0%)
2	B	0.70	1/2662 (0.0%)	0.76	0/3619
2	D	0.70	0/2631	0.77	1/3577 (0.0%)
All	All	0.68	1/11723 (0.0%)	0.76	4/15877 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	138	CYS	CB-SG	-5.33	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	363	LEU	CA-CB-CG	9.10	136.23	115.30
1	A	363	LEU	CA-CB-CG	5.62	128.24	115.30
1	C	180	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	D	136	TRP	CA-CB-CG	5.01	123.23	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3135	0	3024	21	0
1	C	3143	0	3036	32	0
2	B	2597	0	2562	13	0
2	D	2566	0	2531	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	22	4	0
5	C	31	0	22	4	0
6	B	6	0	8	0	0
6	D	12	0	16	0	0
7	A	291	0	0	2	0
7	B	243	0	0	0	0
7	C	297	0	0	7	0
7	D	238	0	0	0	0
All	All	12596	0	11221	65	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (65) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:155[A]:ARG:NH1	7:A:2137:HOH:O	1.99	0.94
1:C:183:ALA:HB1	1:C:185[B]:ARG:HD3	1.53	0.90
1:C:155[A]:ARG:NH1	7:C:2141:HOH:O	1.84	0.89
2:B:146:HIS:ND1	1:C:146[A]:MET:HE1	1.99	0.78
1:A:185:ARG:HG2	7:A:2076:HOH:O	1.86	0.75
1:C:146[A]:MET:HE1	7:C:2146:HOH:O	1.89	0.73
1:C:52:LEU:HD22	1:C:56[A]:LYS:HD3	1.70	0.73
1:C:387:GLN:NE2	7:C:2286:HOH:O	2.22	0.71
1:C:185[B]:ARG:HG2	7:C:2091:HOH:O	1.90	0.70
1:C:146[A]:MET:CE	7:C:2146:HOH:O	2.41	0.67
2:B:274:ARG:NH1	2:B:339:MET:O	2.28	0.67
1:C:82:ARG:HD3	1:C:353:GLU:OE2	1.95	0.66
1:C:313:ASP:OD1	1:C:318:ARG:NH1	2.25	0.66
2:B:74:LEU:HD11	5:C:1403:THV:H4A3	1.80	0.62
5:C:1403:THV:H4'1	5:C:1403:THV:C8	2.12	0.62
1:A:290:HIS:HD2	1:A:297:SER:H	1.46	0.61
1:A:275:GLU:OE1	1:A:277:GLN:NE2	2.34	0.60
2:B:296:GLN:HG3	2:D:296:GLN:HG3	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:275:GLU:OE1	1:C:277:GLN:NE2	2.38	0.56
2:D:55:ARG:HH21	2:D:195:ARG:HD2	1.71	0.56
2:B:289[B]:SER:OG	2:B:309:ARG:NH1	2.39	0.56
1:C:134:TYR:CZ	1:C:353:GLU:HG2	2.41	0.55
1:A:64:MET:HG3	1:A:97:VAL:HG21	1.89	0.54
1:A:23:ILE:HD11	1:C:31:ILE:HG23	1.89	0.53
1:C:351:GLN:HG2	1:C:355:LYS:HE3	1.91	0.52
5:A:1403:THV:C8	5:A:1403:THV:H4'1	2.23	0.51
2:B:146:HIS:ND1	1:C:146[A]:MET:CE	2.75	0.49
1:A:313:ASP:OD2	1:A:318:ARG:CD	2.61	0.48
5:A:1403:THV:H4A3	2:D:74:LEU:HD11	1.96	0.48
1:A:170:GLN:O	2:B:85:GLY:HA3	2.14	0.48
1:A:313:ASP:OD2	1:A:318:ARG:HD3	2.14	0.48
1:C:147:PRO:O	1:C:148:VAL:HG22	2.14	0.47
1:A:186:VAL:HG11	1:A:269:ARG:HG3	1.95	0.47
1:C:64:MET:HG3	1:C:97:VAL:HG21	1.96	0.47
1:C:146[A]:MET:HE2	1:C:146[A]:MET:HB2	1.69	0.46
1:A:39:ARG:HA	1:A:318:ARG:HD2	1.96	0.46
2:B:115:ALA:HB2	2:B:160:ILE:HG23	1.96	0.46
1:C:152:CYS:SG	1:C:155[B]:ARG:HG3	2.57	0.45
1:A:23:ILE:CD1	1:C:31:ILE:HG23	2.46	0.44
1:A:290:HIS:CD2	1:A:297:SER:H	2.31	0.44
2:B:222:VAL:HG11	2:B:336:LEU:HD11	1.98	0.44
1:A:107:ASP:CG	1:A:186:VAL:HG12	2.38	0.44
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.77	0.44
1:C:285:THR:HB	1:C:286:TYR:H	1.57	0.44
1:C:168:ILE:HG22	1:C:204:GLY:HA3	2.00	0.43
2:D:222:VAL:HG11	2:D:336:LEU:HD11	2.00	0.43
5:C:1403:THV:O9	5:C:1403:THV:H351	2.19	0.43
1:C:185[B]:ARG:CG	7:C:2091:HOH:O	2.60	0.43
1:A:48:GLU:HG3	1:C:18:ASP:O	2.19	0.43
2:B:143:ALA:HB3	1:C:146[A]:MET:HG3	2.01	0.42
1:A:291:HIS:CE1	5:A:1403:THV:S1	3.12	0.42
1:C:198:GLU:OE2	5:C:1403:THV:H2A3	2.20	0.42
2:B:146:HIS:CE1	1:C:146[A]:MET:HE1	2.52	0.42
5:A:1403:THV:H352	2:D:98:GLN:OE1	2.20	0.42
1:A:146[B]:MET:HG3	1:A:149:HIS:CE1	2.54	0.41
1:C:314:HIS:CG	1:C:315:PRO:HD2	2.55	0.41
1:C:140:LEU:HA	1:C:140:LEU:HD23	1.88	0.41
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.82	0.41
1:C:78:GLN:OE1	1:C:293:THR:HB	2.20	0.41
1:A:324:LEU:HD23	1:A:329:TRP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:109:GLN:O	2:B:113:GLU:HB2	2.20	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.96	0.41
2:B:165:PRO:HD2	2:B:188:PHE:O	2.20	0.41
1:C:146[A]:MET:HG2	7:C:2066:HOH:O	2.22	0.40
1:C:130:MET:HB3	1:C:352:ALA:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/400 (97%)	379 (98%)	6 (2%)	3 (1%)	27	12
1	C	388/400 (97%)	379 (98%)	6 (2%)	3 (1%)	27	12
2	B	333/350 (95%)	322 (97%)	10 (3%)	1 (0%)	50	36
2	D	329/350 (94%)	317 (96%)	12 (4%)	0	100	100
All	All	1438/1500 (96%)	1397 (97%)	34 (2%)	7 (0%)	38	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	C	113	TYR
1	A	148	VAL
1	C	148	VAL
1	C	226	ILE
1	A	226	ILE
2	B	196	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of

similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/336 (98%)	326 (99%)	2 (1%)	92	92
1	C	328/336 (98%)	324 (99%)	4 (1%)	82	78
2	B	282/295 (96%)	277 (98%)	5 (2%)	71	63
2	D	278/295 (94%)	272 (98%)	6 (2%)	64	54
All	All	1216/1262 (96%)	1199 (99%)	17 (1%)	78	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	296	ASP
2	B	23	LEU
2	B	37	LYS
2	B	50	PHE
2	B	117	TYR
2	B	296	GLN
1	C	29	SER
1	C	186	VAL
1	C	363	LEU
1	C	376	ARG
2	D	24	PHE
2	D	35	LEU
2	D	50	PHE
2	D	117	TYR
2	D	199	GLU
2	D	296	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	HIS
1	A	333	GLN
1	C	387	GLN
2	D	212	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	THV	A	1403	3	31,32,32	2.71	9 (29%)	40,48,48	2.18	9 (22%)
6	GOL	B	1344	-	5,5,5	0.31	0	5,5,5	0.49	0
5	THV	C	1403	3	31,32,32	2.54	8 (25%)	40,48,48	2.02	10 (25%)
6	GOL	D	1344	-	5,5,5	0.18	0	5,5,5	0.46	0
6	GOL	D	1345	-	5,5,5	0.40	0	5,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	THV	A	1403	3	-	0/21/25/25	0/2/2/2
6	GOL	B	1344	-	-	0/4/4/4	0/0/0/0
5	THV	C	1403	3	-	0/21/25/25	0/2/2/2
6	GOL	D	1344	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1345	-	-	0/4/4/4	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1403	THV	C9-C8	11.32	1.56	1.42
5	C	1403	THV	C9-C8	11.20	1.55	1.42
5	A	1403	THV	C35-C5'	4.23	1.60	1.51
5	A	1403	THV	PB-O3A	3.95	1.67	1.60
5	C	1403	THV	PB-O3A	3.50	1.66	1.60
5	A	1403	THV	C5-C4	3.36	1.40	1.36
5	A	1403	THV	C4A-C4	3.19	1.56	1.49
5	C	1403	THV	C5-C4	3.13	1.40	1.36
5	C	1403	THV	C35-C5'	2.91	1.57	1.51
5	A	1403	THV	C5A-C5	2.75	1.54	1.51
5	A	1403	THV	C4'-N3'	2.73	1.39	1.35
5	C	1403	THV	C5A-C5	2.69	1.54	1.51
5	C	1403	THV	C4A-C4	2.46	1.55	1.49
5	A	1403	THV	C2'-N3'	2.27	1.38	1.34
5	C	1403	THV	C4'-N3'	2.25	1.38	1.35
5	C	1403	THV	C2'-N3'	2.13	1.38	1.34
5	A	1403	THV	C2-S1	2.07	1.76	1.73

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1403	THV	C4-N3-C2	7.33	116.17	109.76
5	C	1403	THV	C4-N3-C2	6.70	115.62	109.76
5	A	1403	THV	C2A-C2'-N1'	5.16	123.17	117.02
5	C	1403	THV	C2A-C2'-N1'	4.53	122.42	117.02
5	A	1403	THV	N1'-C2'-N3'	-4.25	117.98	125.65
5	C	1403	THV	C4-C5-S1	-3.94	106.52	110.69
5	A	1403	THV	C5-C4-N3	3.64	115.27	107.66
5	A	1403	THV	C5A-C5-C4	3.63	130.08	127.44
5	A	1403	THV	C4-C5-S1	-3.61	106.87	110.69
5	C	1403	THV	N1'-C2'-N3'	-3.54	119.26	125.65
5	C	1403	THV	C5-C4-N3	3.44	114.85	107.66
5	A	1403	THV	C6'-N1'-C2'	3.30	121.48	115.68
5	C	1403	THV	C4A-C4-C5	-3.23	121.03	129.10
5	C	1403	THV	C6'-N1'-C2'	3.16	121.24	115.68
5	C	1403	THV	C5A-C5-C4	3.04	129.65	127.44
5	A	1403	THV	C4A-C4-C5	-2.76	122.21	129.10
5	A	1403	THV	C5'-C35-N3	-2.38	109.23	113.26
5	C	1403	THV	C5A-C5-S1	2.31	123.81	120.74
5	C	1403	THV	C5'-C35-N3	-2.23	109.48	113.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/400 (95%)	-0.10	20 (5%) 26 26	6, 15, 32, 52	0
1	C	383/400 (95%)	-0.12	18 (4%) 30 30	6, 14, 32, 47	0
2	B	330/350 (94%)	-0.34	5 (1%) 70 71	6, 11, 29, 41	0
2	D	330/350 (94%)	-0.34	6 (1%) 65 66	6, 12, 28, 38	0
All	All	1426/1500 (95%)	-0.21	49 (3%) 43 43	6, 13, 31, 52	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	ALA	5.9
1	A	298	SER	5.4
1	A	299	ALA	5.2
1	A	296	ASP	4.8
1	C	298	SER	4.7
2	D	14	GLU	4.7
2	B	14	GLU	4.5
1	C	300	TYR	4.1
2	B	15	TYR	4.1
1	C	183	ALA	4.1
1	A	297	SER	4.0
1	A	300	TYR	3.8
1	C	400	LYS	3.8
1	C	297	SER	3.6
1	C	294	SER	3.4
1	C	290	HIS	3.3
1	A	183	ALA	3.3
2	B	197	ALA	3.3
1	C	28	ILE	3.3
1	A	313	ASP	3.1
1	C	6	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	28	ILE	3.1
1	A	289	GLY	3.0
1	C	182	ASN	3.0
1	C	288	ILE	2.8
1	C	296	ASP	2.8
2	D	15	TYR	2.7
1	A	26	ASN	2.7
1	A	6	LYS	2.7
1	C	286	TYR	2.7
1	A	182	ASN	2.7
1	C	313	ASP	2.7
1	A	293	THR	2.5
2	D	243	GLU	2.5
2	B	196	ALA	2.4
2	D	197	ALA	2.4
1	A	387	GLN	2.3
1	C	24	GLN	2.3
2	D	301	LEU	2.2
1	C	289	GLY	2.2
1	A	290	HIS	2.2
1	C	40	GLN	2.2
1	A	286	TYR	2.1
2	D	195	ARG	2.1
1	A	331	GLU	2.1
1	A	184	ASN	2.0
1	A	8	GLN	2.0
2	B	301	LEU	2.0
1	A	24	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	D	1345	6/6	0.17	5.49	23,30,32,34	0
4	K	C	1402	1/1	0.07	0.11	18,18,18,18	0
5	THV	C	1403	31/31	0.07	-0.18	6,10,19,23	0
4	K	B	1343	1/1	0.07	-0.39	19,19,19,19	0
5	THV	A	1403	31/31	0.07	-0.58	6,10,18,22	0
4	K	D	1343	1/1	0.06	-0.69	21,21,21,21	0
6	GOL	D	1344	6/6	0.06	-0.77	12,15,18,19	0
3	MN	A	1401	1/1	0.06	-0.94	17,17,17,17	0
6	GOL	B	1344	6/6	0.05	-1.00	15,15,16,17	0
4	K	A	1402	1/1	0.05	-1.18	17,17,17,17	0
3	MN	C	1401	1/1	0.05	-1.39	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.